Excited states of a dilute Bose-Einstein condensate in a harmonic trap

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(February 1, 2008)

The low-lying hydrodynamic normal modes of a dilute Bose-Einstein gas in an isotropic harmonic trap determine the corresponding Bogoliubov amplitudes. In the Thomas-Fermi limit, these modes have large low-temperature occupation numbers, and they permit an explicit construction of the dynamic structure function $S(\mathbf{q},\omega)$. The total noncondensate number $N'(0)$ at zero temperature increases like R^6, where R is the condensate radius measured in units of the oscillator length. The lowest dipole modes are constructed explicitly in the Bogoliubov approximation.

03.75.Fi, 05.30.Jp, 32.80.Pj, 67.40.Db

arXiv:cond-mat/9704234v1 [cond-mat.stat-mech] 28 Apr 1997

I. INTRODUCTION

Recent low-temperature experiments have observed Bose-Einstein condensation in alkali atoms confined to harmonic potentials [1–3]. Subsequent investigations have detected the first few low-lying collective modes of the condensate [4,5]. These results have stimulated a great deal of theoretical activity pertaining to trapped dilute Bose systems. Most of this work relies on the Bogoliubov approximation [6,7], which assumes that only a small fraction of the particles are excited out of the condensate. Clearly such a description fails completely at the onset temperature T_0 for Bose condensation, where the condensate occupation number $N_0(T)$ vanishes, but it does provide a very useful description of the low-temperature behavior of a dilute condensed Bose gas.

In a typical experiment of Refs. [1,2], the condensate is "large," in the sense that its diameter R_0 far exceeds the characteristic width $d_0 = \sqrt{\hbar/m\omega_0}$ of the single-particle ground state of the harmonic trap. (Typically, $d_0 \sim 1$ μm for the traps of Refs. [1,2].) This result can be easily seen by comparing the relative contributions of the kinetic energy, the trap potential energy, and the interaction potential energy to the total energy of the gas. The mean kinetic energy $\langle T\rangle_0 \sim N_0(\hbar^2/2mR_0^2)$ diminishes as the condensate grows, whereas both the mean single-particle confinement energy $\langle V\rangle_0$ and the mean two-particle interaction energy (*i.e.,* the Hartree energy) $\langle V_H\rangle_0$ increase with condensate size. (The subscript 0 denotes an expectation value in the selfconsistent condensate.) For a large condensate, the kinetic energy is then much smaller than both the potential energies. Neglecting the kinetic energy in comparison with the two potential energies gives rise to the so-called "Thomas-Fermi" (TF) approximation, which provides a simple description [8] of the spatially varying condensate density $n_0(\mathbf{r})$.

The two-body repulsion between atoms can be characterized by an s-wave scattering length $a > 0$, or equivalently an s-wave pseudopotential $g = 4\pi\hbar^2 a/m$. The characteristic Hartree energy of the condensate is then $\langle V_H\rangle_0 \sim gN_0^2/R_0^3 \sim \hbar^2 aN_0^2/mR_0^3$. In the Thomas-Fermi limit, this Hartree energy must dominate the kinetic energy $\langle T\rangle_0$. Their ratio defines an important dimensionless quantity

$$\eta_0 \equiv \frac{N_0 a}{d_0} \sim \frac{\langle V_H\rangle_0}{\langle T\rangle_0}. \tag{1}$$

The TF limit therefore requires not only a macroscopically occupied condensate ($N_0 \gg 1$), but also the more stringent condition [8] $\eta_0 = N_0 a/d_0 \gg 1$.

In the Thomas-Fermi limit, the characteristic radius R_0 of the condensate is determined by the balance of $\langle V_H\rangle_0 \sim \hbar^2 aN_0^2/mR_0^3$ and the trap potential $\langle V\rangle_0$, which varies as $\sim N_0(m\omega_0^2 R_0^2)$ for a harmonic confining potential. Minimizing $\langle V + V_H\rangle$ with respect to R_0 yields $N_0 \sim R_0^5/(d_0^4 a)$. Introducing the dimensionless condensate radius $R \equiv R_0/d_0$, we find $\eta_0 \sim R^5$ in the Thomas-Fermi limit.

The collective spectrum of a confined cloud of Bose condensed atoms differs qualitatively from that of a droplet of liquid helium of comparable dimensions. The helium droplet has nearly uniform density except near a thin surface layer. Its bulk collective modes are simply the compressional sound modes of a uniform fluid, whose quantization is set by the boundary conditions at the surface of the drop. For a drop of radius R_0, the minimum wavenumber of a phonon varies as $1/R_0$, and the energy spacing between the collective modes is therefore of order $\hbar s/R_0$, where s is

the bulk speed of sound. As the drop size grows, the minimum excitation energy tends to zero for a large drop, and the spectrum approaches the gapless spectrum of bulk helium, as expected.

In a confined compressible atomic gas, however, the density of the condensate varies with the size of the cloud, in contrast with the nearly constant density of a drop of liquid. We have seen that, in the Thomas-Fermi limit, a cloud of radius R_0 contains $N_0 \sim R^5(d_0/a)$ condensed atoms. The mean density of the condensate is then $N_0/R_0^3 \sim R^2$.

The speed of sound in a dilute Bose gas varies as the square root of its density [6], so that $s \sim R$. The typical energy spacing between quantized sound modes in a harmonically confined cloud then varies as $s/R \sim R^0$. Thus while the maximum wavelength grows linearly with the size of the cloud, the increased density of a larger cloud raises the speed of sound proportionally, and the minimum excitation frequency is independent of the radius of the cloud [8,11].

The excited states of spatially inhomogeneous Bose condensates can be studied by two equivalent approaches. The original work of Bogoliubov [6] emphasized the underlying quantum character of the problem. His treatment of the uniform condensate is readily generalized to the nonuniform case to yield the Bogoliubov equations [9,10] that constitute the quantum-mechanical Schrödinger equations for a pair of coupled amplitude functions. The eigenvalues of this problem are the energies of the elementary excitations of the Bose condensate; the corresponding amplitudes determine the spatially varying noncondensate density.

More recently, a hydrodynamic approach has proved valuable in determining both the excitation frequencies and the normal-mode amplitudes for the low-lying excited states of a Bose condensate in a harmonic trap in the Thomas-Fermi limit [11]. It is not difficult to prove that these two descriptions are completely equivalent in the Bogoliubov approximation [12,13]. The present work exploits this feature to determine the contribution of the low-lying collective modes to the zero-temperature noncondensate density. In particular, the occupation number of these low-lying modes is large in the TF limit, and a reasonable cutoff for the sum over all such modes suggests that the total noncondensate number N' then scales as R^6 in this limit. Since N_0 scales with R^5, the Bogoliubov approximation that $N' \ll N_0$ necessarily fails for sufficiently large R (or N).

We review the basic formalism in Sec. II and summarize the equivalence between the Bogoliubov and hydrodynamic descriptions in Sec. III, along with the physical properties of the noncondensate. The TF solution for the hydrodynamic normal modes is reviewed briefly in Sec. IV. In Sec. V we use the resulting eigenmodes to determine the corresponding Bogoliubov amplitudes and low-temperature noncondensate occupation. Finally, in Sec. VI, we use the eigenmodes to construct the dynamic structure function $S(\mathbf{q},\omega)$ in the TF limit. An Appendix contains an explicit construction of the exact lowest dipole modes of an interacting Bose gas as well as the corresponding modes in the Bogoliubov approximation.

II. BASIC FORMALISM

We briefly review the Bogoliubov approximation for a nonuniform condensed Bose gas, which was introduced independently by Gross [14] and Pitaevskii [15] to study vortices and their excitations. (In this context, the condensate has a uniform density n_0 except in the immediate vicinity of the vortex core.)

At low densities, the two-particle interaction potential may be replaced by a short-range pseudopotential with $V(\mathbf{r}) \approx g\delta(\mathbf{r})$, where g is expressed in terms of the s-wave scattering length a through the relation $g = 4\pi a\hbar^2/m$ [16]. The present work considers only "repulsive" interactions with $g, a > 0$.

For a uniform condensate with density n_0, a small deformation of the condensate wave function with spatial scale λ involves a squared gradient (*i.e.,* kinetic) energy $\sim \hbar^2/2m\lambda^2$. It is useful to define a "coherence" (or "correlation") length

$$\xi \equiv \frac{1}{\sqrt{8\pi a n_0}} \tag{2}$$

through the balance between this kinetic energy and the repulsive interparticle potential energy gn_0. The coherence length becomes arbitrarily large for an ideal Bose gas (*i.e.,* when $a \to 0$).

In the Bogoliubov approximation, the fractional depletion of the condensate N'/N is of order [6,7] $\sqrt{n_0 a^3}$. For the Bogoliubov approximation to be valid, N'/N must be small, which implies the number of particles per scattering volume $n_0 a^3$ is much smaller than unity. (This condition is strongly violated in liquid ^{4}He.) Equivalently, we require that $\xi/a \sim (n_0 a^3)^{-1/2}$ be much greater than unity.

The presence of an external trap introduces another length R_0 that characterizes the spatial size of the condensate. If $\xi \gg R_0$, then the system resembles an ideal Bose gas with negligible interactions. If $\xi \ll R_0$, however, the system differs qualitatively from an ideal Bose gas. In the experiments on Bose-condensed sodium atoms in Ref. [18], the scattering length is $a \sim 4.9$ nm, the trap has a characteristic oscillator length $d_0 \sim 1.9\ \mu$m, and there are $N_0 \sim 5 \times 10^6$ condensed atoms. The equivalent mean (isotropic) condensate radius $R_0 \sim 20\ \mu$m implies a central condensate number

density $n_0 \sim 4 \times 10^{20}$ m^{-3}. Then $\xi \sim 0.14$ μm $\ll R_0$, and the system is indeed a dilute interacting Bose gas with $a \ll \xi \ll R_0$, definitely far from ideal.

For simplicity, we consider here only a spherical harmonic trap, with

$$V(\mathbf{r}) = \tfrac{1}{2} m\omega_0^2 r^2, \tag{3}$$

and a characteristic length scale

$$d_0 = \sqrt{\frac{\hbar}{m\omega_0}} \tag{4}$$

corresponding to the Gaussian width of the single-particle ground state of a single particle of mass m in the trap. When the trap contains a large number N_0 of condensed particles, their mutual repulsion causes the cloud of atoms to expand. The actual condensate density $\sim N_0/R_0^3$ is then much smaller than the simple estimate $\sim N_0/d_0^3$. Specifically, when the Thomas-Fermi parameter $\eta_0 \equiv N_0 a/d_0$ is sufficiently large, the dimensionless radial expansion factor $R \equiv R_0/d_0$ is [8] $(15\eta_0)^{1/5}$. This reduction in the particle density (by a factor of order $\eta_0^{-3/5}$) means that the system remains dilute for $\eta_0^{2/5}(a/d_0)^2 \ll 1$. Put another way, N_0 must be much less than $(d_0/a)^6$, which is $\sim 10^{15}$ for Bose-condensed sodium atoms in Ref. [18].

A spatially nonuniform Bose condensate is characterized by a condensate wave function $\Psi(\mathbf{r})$ that can be normalized to the total number of condensate particles, *i.e.,* $\int d^3r\,|\Psi|^2 = N_0$. Then $n_0(\mathbf{r}) = |\Psi(\mathbf{r})|^2$ is the condensate particle density. For a dilute Bose gas at low temperature, Ψ obeys a selfconsistent nonlinear Schrödinger equation known as the Gross-Pitaevskii (GP) equation [14,15]

$$(T + V + V_H - \mu)\Psi = 0, \tag{5}$$

where $T = -\hbar^2\nabla^2/2m$ is the kinetic-energy operator, $V(\mathbf{r})$ is the trap potential energy operator, $V_H(\mathbf{r}) = g|\Psi(\mathbf{r})|^2 = gn_0(\mathbf{r})$ specifies the mean (Hartree) pseudopotential due to the condensate, and μ is the chemical potential. For a stationary condensate, Ψ can be taken as real, but the generalization to a complex condensate wave function $\Psi = e^{iS}\,|\Psi|$ with superfluid velocity $\mathbf{v}_s = (\hbar/m)\,\nabla S$ is not difficult. (Such a complex condensate could describe, for example, a vortex [9,12,14,15].)

If the mean condensate kinetic energy $\langle T\rangle_0 \equiv \int d^3r\,\Psi^*\,T\,\Psi$ is negligible compared to the potential energies $\langle V_H\rangle_0$ and $\langle V\rangle_0$ [8], which holds for $\eta_0 \gg 1$, then the Gross-Pitaevskii equation [Eq. (5)] can be approximated by its last three terms. In this limit, for each spatial position $\mathbf{r}$, either the condensate wave function vanishes or the condensate density satisfies the "Thomas-Fermi" approximation

$$V_H(\mathbf{r}) = gn_0(\mathbf{r}) = \big[\mu - V(\mathbf{r})\big]\,\theta\big[\mu - V(\mathbf{r})\big], \tag{6}$$

where $\theta(x)$ denotes the unit positive step function. For a spherical harmonic trap with oscillator length d_0 and oscillator frequency ω_0, the TF condensate density is an inverted parabola that vanishes beyond a dimensionless cutoff radius $R \approx (15\eta_0)^{1/5}$ defined in terms of the chemical potential $\mu = \frac{1}{2}\hbar\omega_0 R^2$ [8].

The validity of this TF approximation has been investigated both numerically for various values of the dimensionless parameter R [19,20] and analytically [21] through an expansion in powers of the "small" parameter $1/R^4$. This latter treatment shows that the TF approximation fails in a thin surface region of thickness $\sim d_0(d_0/R_0)^{1/3} \sim d_0 R^{-1/3}$, where the formally negligible correction terms eliminate the singularity of $|d\Psi_{\rm TF}/dr|^2$ at the condensate surface. As a result, the condensate kinetic energy acquires a logarithmic correction of order $(\hbar\omega_0/2R^2)\ln R$.

In an ideal Bose gas at zero temperature, all the particles are condensed in the single-particle ground state of the trap. Repulsive interactions excite a (small) fraction N'/N of the particles out of the condensate, even at zero temperature. These excited particles occupy the various normal-mode eigenstates that satisfy the (linear) Bogoliubov equations [6,9,10,12,15]

$$\mathcal{L}u_j - V_H v_j = E_j u_j, \tag{7a}$$

$$-\,V_H u_j + \mathcal{L}v_j = -E_j v_j, \tag{7b}$$

for the coupled eigenfunctions $u_j(\mathbf{r})$ and $v_j(\mathbf{r})$, and the associated eigenvalues E_j. Here, j denotes a complete set of quantum numbers, and the operator $\mathcal{L}$ has the form

$$\mathcal{L} = T + V + 2V_H - \mu, \tag{8}$$

where we again restrict our attention to stationary condensates. (The generalization to the case of nonzero superfluid velocity is not difficult [12].) In these Bogoliubov equations, the minus sign in the coupling terms is conventionally chosen to ensure that the ratio of the two amplitudes is positive for a uniform Bose gas, where plane waves are the appropriate eigenfunctions: $u_k e^{i\mathbf{k}\cdot\mathbf{r}}$ and $v_k e^{i\mathbf{k}\cdot\mathbf{r}}$. These coupled Schrödinger equations for the amplitudes u_j and v_j are analogous to the multicomponent Dirac equation. (The eigenvalues of the Bogoliubov equations come in $\pm$ pairs; the eigenfunctions of these pairs are related by a simple symmetry relation [9].)

For a localized trapped condensate in an unbounded confining potential, the condensate density n_0 and the two-particle Hartree potential V_H both vanish at infinity, and the amplitudes obey the usual quantum-mechanical bound-state boundary condition that u_j and v_j vanish for $r \to \infty$. Furthermore, for positive eigenvalues, the eigenfunctions can be chosen to satisfy the orthonormality condition [9]

$$\int d^3r \, (u_j^* u_k - v_j^* v_k) = \delta_{jk}. \tag{9}$$

The (low-temperature) total noncondensate number $N'(T)$ is obtained by summing over all eigenstates

$$N'(T) = {\sum_j}' N'_j(T), \tag{10}$$

where the primed sum omits the lowest eigenstate (which simply describes the condensate itself). Here $N'_j(T)$ is the spatial integral of the corresponding temperature-dependent noncondensate density

$$n'_j(\mathbf{r}) \equiv |v_j(\mathbf{r})|^2 + \big(|u_j(\mathbf{r})|^2 + |v_j(\mathbf{r})|^2\big)(e^{\beta E_j} - 1)^{-1}. \tag{11}$$

The second term vanishes as $T \to 0$, leaving the integral of first term as the mean occupation number at zero temperature:

$$N'_j(0) = \int d^3r \, |v_j(\mathbf{r})|^2. \tag{12}$$

At nonzero temperature, the condition $N_0(T) = N - N'(T)$ determines the total condensate number, but the present work emphasizes the zero-temperature limit.

It is helpful to recall briefly the special case of a uniform bulk condensate with constant density n_0 [6,22], where the confining potential V is absent and the Hartree interaction energy and condensate chemical potential are equal: $V_H = \mu = g n_0$. The eigenfunctions are plane waves $\propto e^{i\mathbf{k}\cdot\mathbf{r}}$, and the energy eigenvalues have the familiar Bogoliubov form

$$E_k = \sqrt{2T_k V_H + T_k^2} \approx \begin{cases} \hbar s k, & \text{for } k\xi \ll 1, \\ \hbar^2 k^2/2m, & \text{for } k\xi \gg 1, \end{cases} \tag{13}$$

where $T_k = \hbar^2 k^2/2m$ is the kinetic energy and $s = \sqrt{4\pi a \hbar^2 n_0/m^2} = \hbar/\sqrt{2} m\xi$ is the speed of compressional sound.

The corresponding "coherence factors" u_k and v_k determine the mixing of the two components, and obey the bosonic normalization condition $u_k^2 - v_k^2 = 1$ for each $\mathbf{k}$. At zero temperature, the noncondensate occupation of the $\mathbf{k}$th plane-wave mode is simply

$$N'_k(0) = v_k^2 = \frac{1}{2}\left(\frac{T_k + V_H}{E_k} - 1\right) \approx \begin{cases} \sqrt{V_H/8T_k} \approx (2\sqrt{2}\,k\xi)^{-1}, & \text{for } k\xi \ll 1, \\ V_H^2/4T_k^2 \approx \frac{1}{4}(k\xi)^{-4}, & \text{for } k\xi \gg 1. \end{cases} \tag{14}$$

The long-wavelength singularity in $N'_k(0) \propto k^{-1}$ is integrable, and the short-wavelength behavior ensures that the total noncondensate density $n' = (2\pi)^{-3} \int d^3k \, v_k^2 = \frac{8}{3} n_0 \sqrt{n_0 a^3/\pi}$ is not only finite but also small relative to the condensate density. At low temperature, the corresponding additional thermal occupation for the $\mathbf{k}$th state has the form $\Delta N'_k(T) \equiv N'_k(T) - N'_k(0) \propto T/k^2$.

III. EQUIVALENCE WITH HYDRODYNAMIC FORMALISM

We now return to the general inhomogeneous case. To proceed, it is useful to note that the GP equation (5) for the condensate wave function can be rewritten with Eq. (8) as $\mathcal{L}\Psi = V_H \Psi$, which suggests the following transformation of the Bogoliubov amplitudes

$$u_j = \frac{\Psi\, U_j}{\sqrt{N_0}} \qquad \text{and} \qquad v_j = \frac{\Psi\, V_j}{\sqrt{N_0}}. \tag{15}$$

In particular, it is straightforward to verify that

$$\mathcal{L}u_j = \frac{\Psi}{\sqrt{N_0}}\,(\tilde{T} + V_H)U_j, \tag{16}$$

where $\tilde{T}$ is a differential operator defined by

$$\tilde{T}f \equiv -\frac{\hbar^2}{2m|\Psi|^2}\,\nabla\cdot\big(|\Psi|^2\nabla f\big) = -\frac{\hbar^2}{2m\,n_0}\,\nabla\cdot\big(n_0\nabla f\big). \tag{17}$$

To simplify (7) further, define

$$F_j = U_j + V_j \qquad \text{and} \qquad G_j = U_j - V_j; \tag{18}$$

Then the Bogoliubov equations can be rewritten exactly as

$$\tilde{T}F_j = E_j G_j, \tag{19a}$$

$$(\tilde{T} + 2V_H)G_j = E_j F_j. \tag{19b}$$

These two equations can be combined to give a *single* equation for G_j:

$$(\tilde{T}^2 + 2\tilde{T}V_H)G_j = E_j^2 G_j. \tag{20}$$

The corresponding F_j follows from Eq. (19b). Comparison with Eq. (9) shows that the normalization for the jth eigenstate is simply

$$1 = \frac{1}{2N_0}\int d^3r\,|\Psi|^2\,(F_j^* G_j + F_j G_j^*) = \frac{1}{N_0}\int d^3r\,|\Psi|^2\,\Re(F_j^* G_j). \tag{21}$$

The zero-temperature occupation of the jth excited state is then [compare Eq. (11)]

$$N_j'(0) = \frac{1}{4N_0}\int d^3r\,|\Psi|^2\,|F_j - G_j|^2. \tag{22}$$

To make contact with the hydrodynamic description of these same normal modes, recall that the second-quantized operators for the fluctuations in the density $\hat{\rho}'$ and velocity potential $\hat{\Phi}'$ are simply linear combinations of the field operators $\hat{\phi}$ and $\hat{\phi}^\dagger$ [12]. It follows that the corresponding normal-mode amplitudes ρ_j and Φ_j are also linearly related to the Bogoliubov amplitudes u_j and v_j. A straightforward comparison yields

$$\rho_j = \frac{n_0}{\sqrt{N_0}}\,G_j, \tag{23a}$$

$$\Phi_j = \frac{\hbar}{2im\sqrt{N_0}}\,F_j. \tag{23b}$$

Conversely, if the hydrodynamic amplitudes are known, the corresponding Bogoliubov wave functions become

$$u_j = \tfrac{1}{2}\Psi\left(\frac{\rho_j}{n_0} + \frac{2im\,\Phi_j}{\hbar}\right) = \frac{\rho_j}{2\Psi} + \frac{im\,\Psi\,\Phi_j}{\hbar}, \tag{24a}$$

$$v_j = \tfrac{1}{2}\Psi\left(\frac{\rho_j}{n_0} - \frac{2im\,\Phi_j}{\hbar}\right) = \frac{\rho_j}{2\Psi} - \frac{im\,\Psi\,\Phi_j}{\hbar}. \tag{24b}$$

A straightforward combination of Eqs. (19) and (23) immediately reproduces the known hydrodynamic equations for the normal modes of a stationary condensate [11–13]. For example, the product $V_H G_j$ is just the density-fluctuation normal-mode eigenfunction ρ_j itself (apart from a constant factor) and Eq. (20) becomes

$$-\frac{4\pi a\hbar^2}{m^2}\nabla\cdot\big(n_0\nabla\rho_j\big) + \frac{\hbar^2}{4m^2}\nabla\cdot\left\{n_0\nabla\left[\frac{1}{n_0}\nabla\cdot\left(n_0\nabla\,\frac{\rho_j}{n_0}\right)\right]\right\} = \omega_j^2\rho_j, \tag{25}$$

where $\omega_j = E_j/\hbar$ is the normal-mode eigenfrequency.

IV. LOW-LYING NORMAL-MODE HYDRODYNAMIC AMPLITUDES IN TF LIMIT

It is convenient to rewrite the Bogoliubov equations in terms of suitably rescaled variables. We let $\mathbf{x} \equiv \mathbf{r}/R_0$ be the dimensionless position vector, where R_0 is the characteristic condensate radius, and introduce the dimensionless condensate wave function

$$\chi = \left(4\pi\tilde{\eta}_0 \frac{R_0^3}{N_0}\right)^{1/2} \Psi, \tag{26}$$

where the quantity in parentheses is roughly the volume per condensate particle. The rescaled condensate wave function χ satisfies the dimensionless radial normalization condition $\int_0^\infty x^2\,dx\,|\chi|^2 = \tilde{\eta}_0$, where the dimensionless parameter $\tilde{\eta}_0$ in Eq. (26) is defined by

$$\tilde{\eta}_0 \equiv \frac{\eta_0}{R^5} = \frac{N_0 a d_0^4}{R_0^5}. \tag{27}$$

In the Thomas-Fermi limit, $\tilde{\eta}_0$ becomes independent of the size of the condensate. To complete our scaling of variables, we express all energies in units of $\hbar\omega_0$.

The three relevant operators then become

$$\tilde{T} = -\frac{1}{2R^2\,|\chi|^2}\,\nabla_{\mathbf{x}}\cdot\left(|\chi|^2\nabla_{\mathbf{x}}\right), \tag{28a}$$

$$V = \tfrac{1}{2}R^2\,x^2, \tag{28b}$$

$$V_H = R^2|\chi|^2. \tag{28c}$$

These expressions clearly exhibit the dependence on the large parameter R^2 and show that the trap and Hartree energies are comparable to one another and both much larger than the kinetic energy. In the rescaled variables, the product $\tilde{T}V_H$ is independent of R, and the basic eigenvalue Eq. (25) for the hydrodynamic normal-mode amplitude ρ_j becomes

$$-\nabla_{\mathbf{x}}\cdot\left(|\chi|^2\nabla_{\mathbf{x}}\,\rho_j\right) + \frac{1}{4}\,\epsilon\,\nabla_{\mathbf{x}}\cdot\left\{|\chi|^2\nabla_{\mathbf{x}}\left[\frac{1}{|\chi|^2}\nabla_{\mathbf{x}}\cdot\left(|\chi|^2\nabla_{\mathbf{x}}\,\frac{\rho_j}{|\chi|^2}\right)\right]\right\} = E_j^2\rho_j, \tag{29}$$

where E_j is the dimensionless energy (or frequency) of the jth normal mode, and $\epsilon \equiv R^{-4}$ is the appropriate small expansion parameter.

For a spherical trap, Baym and Pethick [8] showed that $\tilde{\eta}_0 \approx \frac{1}{15}$ in the TF limit, and the rescaled condensate wave function is simply [8]

$$|\chi|^2 \approx \chi_0^2 = \frac{1}{2}(1-x^2)\,\theta(1-x), \tag{30}$$

where x is the scaled radial variable. For a spherical trap, the eigenfunctions of Eq. (29) can be written as a product of (real) radial functions $\rho_{nl}(x)$ and a spherical harmonic $Y_{lm}(\theta,\phi)$, where $j = (nlm)$, and n is the radial quantum number.

Stringari [11] has solved Eq. (29) in the TF limit (*i.e.,* to zeroth order in ϵ) and has shown that the eigenfunctions and eigenvalues are independent of R, as discussed in Sec. I. In particular, the TF energy eigenvalue is given by

$$E_{nl}^2 = l + n(2n+2l+3) = \alpha - \tfrac{1}{2} + 2n(n+\alpha+1). \tag{31}$$

where $\alpha \equiv l + \frac{1}{2}$ is half an odd integer. The corresponding radial functions $\rho_{nl}(x)$ have the form $x^l P_{nl}(x^2)$, where $P_{nl}(x^2)$ are nth-order polynomials in x^2. It is not difficult to verify that these polynomials satisfy the hypergeometric equation [23] with the explicit (unnormalized) form

$$P_{nl}(u) = F(-n, n+\alpha+1; \alpha+1; u) = \frac{\Gamma(\alpha+1)}{\Gamma(n+\alpha+1)}\,u^{-\alpha}\,\frac{d^n}{du^n}\left[\,u^{n+\alpha}\,(1-u)^n\,\right]; \tag{32}$$

the first two such polynomials are $P_{0l} = 1$ and $P_{1l} = 1 - (\alpha+2)u/(\alpha+1) = 1 - (2l+5)u/(2l+3)$.

The polynomials P_{nl} are a special class of Jacobi polynomials, with $P_{nl}(u) \propto P_n^{(\alpha,0)}(1-2u)$. For any l, they form an orthonormal set on the interval $0 \le u \le 1$ with weight u^α. An n-fold integration by parts with the explicit differential expression in Eq. (32) readily yields the radial normalization integral

$$I^0_{nl} = \int_0^1 x^2\,dx\,\big[\rho_{nl}(x)\big]^2 = \tfrac{1}{2}\int_0^1 du\,u^\alpha\,\big[P_{nl}(u)\big]^2 = \left[\frac{\Gamma(\alpha+1)\,n!}{\Gamma(n+\alpha+1)}\right]^2 \frac{1}{2(2n+\alpha+1)}\,, \tag{33}$$

which also follows directly from the properties of the Jacobi polynomials [23].

The transformation introduced in Eq. (15) explicitly eliminates the chemical potential from the Bogoliubov equations for the amplitudes u_j and v_j. As shown above, it leads to the hydrodynamic Eq. (29) that involves only the condensate density. In principle, the Bogoliubov description is wholly equivalent to this hydrodynamic description, but an explicit verification involves higher-order terms in the condensate wave function [25].

To understand the situation in more detail, recall that, in the grand canonical ensemble at zero temperature, the chemical potential μ determines both the total number of particles N and the number $N_0 \le N$ in the condensate [24]. In the present approximation of retaining only the condensate contribution (*i. e.* $N \approx N_0$), the Gross-Pitaevskii equation wholly characterizes the resulting functional dependence $N_0(\mu)$. For large dimensionless μ, this relation is just the familiar TF result plus small corrections [25]. It is straightforward to verify that direct substitution of the TF chemical potential and the TF wave function χ_0 from Eq. (30) into the Bogoliubov equations yields an incorrect eigenvalue spectrum. A more careful treatment that includes the leading correction χ_1 of order $1/R^4$ indeed reproduces the hydrodynamic eigenvalues and eigenfunctions.

V. NONCONDENSATE OCCUPATION AT LOW TEMPERATURE

Stringari's theoretical prediction [11] of the frequencies of the lowest hydrodynamic normal modes rapidly received experimental confirmation [4,5]. The present work extends his results to determine the occupation number of the same low-lying normal modes. This analysis makes essential use of the quantum-mechanical Bogoliubov amplitudes u_{nlm} and v_{nlm} for quasiparticle creation and annihilation operators associated with these particular single-particle states [12,13], and exploits the equivalence between the hydrodynamic and Bogoliubov descriptions.

Equation (23) expresses the radial amplitude G_{nl} directly in terms of ρ_{nl}; apart from a constant factor, we have $G_{nl}(x) \propto \rho_{nl}(x)/|\chi_0(x)|^2$, where $|\chi_0(x)|^2 = \frac{1}{2}(1-x^2)$ is the parabolic TF condensate density profile. In addition, Eqs. (19b) and (28c) show that $F_{nl} \approx 2R^2|\chi_0|^2 G_{nl}/E_{nl}$, apart from corrections that become small as $R \to \infty$. Together, these expressions suggest the following normalization

$$F_{nl}(x) = \frac{2R\,C_{nl}}{E_{nl}}\,\rho_{nl}(x) = \frac{2R\,C_{nl}}{E_{nl}}\,x^l\,P_{nl}(x^2), \tag{34a}$$

$$G_{nl}(x) = \frac{C_{nl}}{R}\,\frac{\rho_{nl}(x)}{|\chi_0(x)|^2} = \frac{C_{nl}}{R}\,\frac{x^l\,P_{nl}(x^2)}{|\chi_0(x)|^2}, \tag{34b}$$

where C_{nl} is a normalization constant determined from Eq. (21). A combination of the previous results leads to the explicit expression

$$C^2_{nl} = \frac{2\pi\tilde{\eta}_0\,E_{nl}}{I^0_{nl}}, \tag{35}$$

which completely determines the radial amplitudes F_{nl} and G_{nl} in the TF limit. Note that while F_{nl} is of order R, G_{nl} is of order $1/R$, so that $U_{nl} = \frac{1}{2}(F_{nl} + G_{nl})$ and $V_{nl} = \frac{1}{2}(F_{nl} - G_{nl})$ are *both* large for the low-lying states of a large condensate. [A similar behavior occurs at long wavelengths ($k\xi \lesssim 1$) for a uniform dilute Bose gas, as seen from the bosonic normalization condition $u_k^2 - v_k^2 = 1$ and Eq. (14).]

The zero-temperature occupation of the low-lying normal modes with quantum numbers nlm follows directly from Eq. (22). The leading term from $|F_{nl}|^2$ is of order R^2, and the cross term between F_{nl} and G_{nl} just reproduces the normalization integral from Eq. (33). It is convenient to introduce the general class of integrals

$$I^j_{nl} \equiv \int_0^1 x^2\,dx\,(1-x^2)^j\,\big[\rho_{nl}(x)\big]^2 = \tfrac{1}{2}\int_0^1 du\,u^\alpha\,(1-u)^j\,\big[P_{nl}(u)\big]^2. \tag{36}$$

For $j = 0$ this quantity is simply the normalization integral considered previously; for $j = 1$, it can be evaluated with repeated integration by parts, leading to the ratio

$$\frac{I^1_{nl}}{I^0_{nl}} = \frac{2n(n+\alpha+1)+\alpha}{(2n+\alpha)(2n+\alpha+2)} = \frac{E^2_{nl}+\frac{1}{2}}{(2n+\alpha)(2n+\alpha+2)}. \tag{37}$$

A combination of these results yields an explicit expression for the zero-temperature occupation of the low-lying excited states of a large isotropic condensate in an isotropic harmonic trap:

$$N'_{nl}(0) \approx \frac{R^2}{4E_{nl}}\,\frac{E^2_{nl}+\frac{1}{2}}{(2n+\alpha)(2n+\alpha+2)} - \tfrac{1}{2}, \tag{38}$$

where the omitted term comes from the radial integral of $|G_{nl}|^2$ and is of order R^{-2}.

Since $R^2 \gg 1$ in the TF limit, the noncondensate occupation $N'_{nl}(0)$ is large for the low-lying states with small n and l, whose dimensionless energy is of order unity. For example, for the lowest dipole mode with $n = 0$, $l = 1$, we have $E_{01} = 1$ and $N'_{01}(0) \approx \frac{1}{14}R^2 - \frac{1}{2}$. This behavior is evidently very similar to that for a uniform dilute Bose gas, where Eq. (14) shows that $N'_k(0) = (2\sqrt{2}\,k\xi)^{-1} \gg 1$ for long wavelengths such that $k\xi \lesssim 1$. Indeed, Eq. (14) also makes clear that the long-wavelength approximation fails when the kinetic energy T_k of the plane-wave state becomes comparable to the Hartree energy V_H, and a similar behavior is expected in the present case of a trapped condensate.

Specifically, the amplitude F_{nl} was obtained from G_{nl} by neglecting $\tilde{T}$ relative to $2V_H$ in Eq. (19b). This approximation holds for radial states with sufficiently few nodes, but it necessarily fails for highly excited states whose large kinetic energy reflects the bending energy associated with rapid oscillations (and hence many nodes) in the wave function [11]. By analogy with the corresponding situation for a uniform Bose gas, it is natural to conjecture that the explicit expression in Eq. (38) is valid only for low-lying modes with $N'_{nl}(0) \gtrsim 1$. Verification of this conjecture would require a detailed study of the highly excited modes of the large condensate; it involves corrections to the TF condensate wave function associated with the boundary layer [21] and a WKB (phase-integral) description of the rapid oscillations inherent in the short-wavelength limit. This difficult analysis remains for future investigation.

The total number N' of noncondensed particles is the sum of N'_j over all eigenstates of the Bogoliubov equations, omitting the lowest solution with zero energy (which describes the condensate itself). In the present case of a spherical condensate at zero temperature, we have

$$N'(0) = {\sum_{nl}}'\,(2l+1)\,N'_{nl}(0), \tag{39}$$

where the factor $2l + 1$ represents the degeneracy associated with the sum over azimuthal quantum numbers m and the prime on the sum indicates that the term $n = l = 0$ is omitted. In the TF limit, the zero-temperature occupation of the low-lying modes is given by Eq. (38). As argued above, the sum must be cut off when $N'_{nl}(0) \approx 1$. (Apart from a numerical factor of order unity, an analogous cutoff gives the correct total noncondensate fraction for a uniform condensate at zero temperature, $N'/N_0 \sim \sqrt{n_0 a^3}$). Stringari [11] has suggested that the TF expression for E_{nl} in Eq. (31) holds for $E_{nl} \lesssim \mu$, which is $\frac{1}{2}R^2$ in the TF limit. It is not hard to see that this criterion provides a qualitatively similar cutoff.

For large R, the N'_{nl} vary slowly with n and l, and the double sum Eq. (39) can be approximated by an integral over continuous variables n and $\alpha \equiv l + \frac{1}{2}$, with

$$N'(0) = {\sum_{nl}}'(2l+1)\,N'_{nl}(0) \approx \int dn \int d\alpha\, 2\alpha \left[\frac{R^2}{4E_{nl}}\,\frac{E^2_{nl}+\frac{1}{2}}{(2n+\alpha)(2n+\alpha+2)} - \tfrac{1}{2}\right], \tag{40}$$

where this double integral runs over the region $N'_{nl} \geq 1$. To clarify its structure, it is convenient to introduce new variables

$$s \equiv n + l + 1 = n + \alpha + \tfrac{1}{2} \qquad \text{and} \qquad t \equiv n + \tfrac{1}{2}, \tag{41}$$

or, equivalently

$$n = t - \tfrac{1}{2} \qquad \text{and} \qquad \alpha = s - t; \tag{42}$$

this transformation has unit Jacobian, and the allowed region in the st plane is the first octant $0 \leq t \leq s$, apart from a small region around the origin. In these new variables, the TF energy eigenvalue in Eq. (31) becomes $E^2 = 2st - 1$, and the corresponding noncondensate occupation number is

$$N'_{nl}(0) \approx \frac{R^2}{4}\,\frac{2st-\frac{1}{2}}{\sqrt{2st-1}}\,\frac{1}{(s+t)^2-1} - \tfrac{1}{2}. \tag{43}$$

To isolate the dominant contribution to the integral in the st plane, it is helpful to introduce plane-polar coordinates (ζ,ϕ), with $s=\zeta\cos\phi$ and $t=\zeta\sin\phi$; for large ζ, the leading behavior is $N'\sim R^2/\zeta$, apart from angular factors. It is not difficult to see that the angular integral over $0\le\phi\le\pi/4$ converges, and the radial integral must be cut off at $\zeta_{\max}\sim R^2$. In this way, the total noncondensate number at zero temperature becomes

$$N'(0) \sim \int_1^{R^2} \zeta^2\, d\zeta\, \frac{R^2}{\zeta} \sim R^6. \tag{44}$$

As shown by Baym and Pethick [8], the number of condensed particles in the TF limit is given by $N_0 \approx \frac{1}{15} d_0 R^5/a$, proportional to R^5. So from Eq. (44), the ratio of uncondensed to condensed particles at zero temperature in the Thomas-Fermi limit is

$$\frac{N'(0)}{N_0} \sim R\frac{a}{d_0}, \tag{45}$$

apart from a numerical constant of order unity. As expected, this is comparable to the uncondensed fraction in a homogeneous Bose gas of density N_0/R_0^3. Since the validity of the Bogoliubov approximation depends on the condition $N'/N_0 \ll 1$, we find that the present description holds only for $R \ll d_0/a$. When combined with Baym and Pethick's result, this condition indicates that the condensate is dilute only for $N_0 \sim R^5(d_0/a) \ll (d_0/a)^6$, in agreement with the condition found in Sec. II.

It is evident from Eqs. (9) and (11) that the zero-temperature eigenvalues and eigenfunctions of the Bogoliubov equations also determine the low-temperature thermal depletion of the condensate through the relation

$$\Delta N'_{nl}(T) = N'_{nl}(T) - N'_{nl}(0) \approx \frac{1+2N'_{nl}(0)}{\exp(\beta\hbar\omega_0 E_{nl})-1}, \tag{46}$$

where $E_{nl}=\sqrt{l+n(2n+2l+3)}$ is the dimensionless energy eigenvalue, here taken from Eq. (31). It is convenient to define a characteristic temperature $\Theta \equiv \hbar\omega_0/k_B$ for thermal excitation of the first excited state; note that Θ is much smaller than the ideal-gas transition temperature $T_0^{(0)} \sim \Theta N^{1/3}$. Furthermore, the actual transition temperature T_0 for a dilute trapped Bose gas is only slightly less than the ideal-gas transition temperature $T_0^{(0)}$, so that $\Theta/T_0 \approx N^{-1/3}$. As a result, the low-temperature thermal occupation of each low-lying mode increases linearly with temperature

$$\Delta N'_{nl}(T) \approx [1+2N'_{nl}(0)]\frac{T}{\Theta\, E_{nl}} \tag{47}$$

for $\Theta\, E_{nl} \ll T \ll T_0$.

VI. DYNAMIC STRUCTURE FACTOR $S(\mathbf{q},\omega)$

Consider an external probe that scatters with momentum transfer $\hbar\mathbf{q}$ and energy transfer $\hbar\omega$ to a target. If the probe couples weakly to the number density of the target (here, the trapped Bose condensed system), the differential cross section $d^2\sigma/d\Omega d\omega$ is proportional to the dynamic structure factor [26,27]

$$S(\mathbf{q},\omega) = \frac{1}{NZ}\sum_{fi} e^{-\beta E_i}\,|\langle f|\tilde{\rho}'^{\dagger}_{\mathbf{q}}|i\rangle|^2\,\delta\Big(\omega - \frac{E_f-E_i}{\hbar}\Big), \tag{48}$$

where i and f refer to exact states of the interacting target with energies E_i and E_f, $Z=\sum_i \exp(-\beta E_i)$ is the target partition function, and $\tilde{\rho}'^{\dagger}_{\mathbf{q}} = \int d^3r\, e^{i\mathbf{q}\cdot\mathbf{r}}\,\hat{\rho}'(\mathbf{r})$ is the "creation operator" for a density fluctuation with wave number $\mathbf{q}$.

In the Bogoliubov approximation, the density-fluctuation operator $\hat{\rho}'(\mathbf{r})$ is proportional to a linear combination of the field operators $\hat{\phi}(\mathbf{r})$ and $\hat{\phi}^{\dagger}(\mathbf{r})$. As a result, Eq. (23a) immediately yields the corresponding expansion in bosonic quasiparticle operators [12] α_j and $\alpha_j^{\dagger}$

$$\hat{\rho}'(\mathbf{r}) = {\sum_j}' \big[\rho_j(\mathbf{r})\alpha_j + \rho_j^*(\mathbf{r})\alpha_j^{\dagger}\big], \tag{49}$$

where ρ_j is essentially a linear combination of the Bogoliubov amplitudes, and the primed sum runs over all the excited states of the condensate. The evaluation of the dynamic structure factor is straightforward, giving the explicit result

$$S(\mathbf{q},\omega) = \frac{1}{N}\sum_j{}' \left[(1+f_j)\,|\tilde\rho_j^*(\mathbf{q})|^2\delta(\omega - E_j/\hbar) + f_j\,|\tilde\rho_j(\mathbf{q})|^2\delta(\omega + E_j/\hbar)\right], \tag{50}$$

where $f_j = \left[\exp(\beta E_j) - 1\right]^{-1}$ is the thermal Bose-Einstein function and $\tilde\rho_j(\mathbf{q})$ is the spatial Fourier transform of $\rho_j(\mathbf{r})$.

For a spherical trap, the amplitudes are given in Eq. (34b). Introducing the dimensionless variable $Q = qR_0$, we readily obtain the following dimensionless dynamic structure factor (scaled with the oscillator frequency ω_0)

$$S(Q,\omega) \approx \frac{1}{2\tilde\eta_0 R^2}\sum_{nl}{}' \frac{(2l+1)E_{nl}}{I_{nl}^0}\,|p_{nl}(Q)|^2\left[(1+f_{nl})\,\delta(\omega - E_{nl}) + f_{nl}\,\delta(\omega + E_{nl})\right], \tag{51}$$

where E_{nl} is the dimensionless energy (or frequency) from Eq. (31) and

$$p_{nl}(Q) = \int_0^1 dx\, x^{l+2}\, P_{nl}(x^2)\, j_l(Qx). \tag{52}$$

Equation (51) makes it easy to verify that this approximate dynamic structure factor obeys the detailed-balance condition [26] $S(-\mathbf{Q},-\omega) = e^{-\beta\hbar\omega}S(\mathbf{Q},\omega)$.

The integral in Eq. (52) can be evaluated with the standard expression for the spherical Bessel function j_l as an l-fold derivative of j_0 [28]

$$\frac{j_l(x)}{x^l} = (-2)^l\,\frac{d^l}{du^l}j_0(x), \tag{53}$$

where $u = x^2$, along with the explicit formula for $P_{nl}(x^2)$ in Eq. (32):

$$p_{nl}(Q) = \frac{\Gamma(\alpha+1)}{\Gamma(n+\alpha+1)}\,\frac{2^{l-1}(-1)^l}{Q^l}\int_0^1 du\,\frac{d^n}{du^n}\left[u^{n+\alpha}(1-u)^n\right]\frac{d^l}{du^l}j_0(Qx). \tag{54}$$

An n-fold integration by parts then yields

$$p_{nl}(Q) = \frac{\Gamma(\alpha+1)}{\Gamma(n+\alpha+1)}\,\frac{Q^{2n+l}}{2^{n+1}}\int_0^1 du\,u^{n+\alpha}\,(1-u)^n\,\frac{j_{n+l}(Qx)}{(Qx)^{n+l}}, \tag{55}$$

which can be integrated term-by-term after expanding the spherical Bessel function as a power series in uQ^2. The resulting series can be re-summed to yield the remarkably simple expression

$$p_{nl}(Q) = \frac{\Gamma(\alpha+1)\,n!}{\Gamma(n+\alpha+1)}\,\frac{j_{2n+l+1}(Q)}{Q}. \tag{56}$$

It is convenient to rewrite the dynamic structure factor as

$$S(Q,\omega) = \sum_{nl}{}' S_{nl}(Q)\left[(1+f_{nl})\,\delta(\omega - E_{nl}) + f_{nl}\,\delta(\omega + E_{nl})\right], \tag{57}$$

where $f_{nl} = [\exp(\Theta E_{nl}/T) - 1]^{-1}$, and

$$S_{nl}(Q) = \frac{(2l+1)\,(2n+l+\frac{3}{2})\,E_{nl}}{\tilde\eta_0 Q^2 R^2}\left[j_{2n+l+1}(Q)\right]^2. \tag{58}$$

For $Q\to 0$, the leading term arises from the dipole-sloshing mode $n=0$, $l=1$, with $S_{01}\approx Q^2/2R^2 + \mathcal{O}(Q^4)$; the next contributions (of order Q^4) arise from the terms with $n=1$, $l=0$ and $n=0$, $l=2$. In addition, the frequency integral is simply the static structure factor

$$\int_{-\infty}^{\infty} d\omega\, S(Q,\omega) = S(Q) = \sum_{nl}{}' S_{nl}(Q)\,\coth\left(\frac{\Theta E_{nl}}{2T}\right), \tag{59}$$

with the long-wavelength limit

$$S(Q) \approx \frac{Q^2}{2R^2} \coth\left(\frac{\Theta}{2T}\right) + \mathcal{O}(Q^4). \tag{60}$$

Finally, the first moment is the f-sum rule [26]

$$\int_{-\infty}^{\infty} d\omega\, \omega\, S(Q,\omega) = \sum_{nl}{}' S_{nl}(Q)\, E_{nl} = \frac{Q^2}{2R^2}\ \Big(= \frac{\hbar^2 q^2}{2m} \text{ in conventional units}\Big). \tag{61}$$

The dipole-sloshing mode exhausts this sum rule at long wavelengths, but it otherwise implies a rather intricate identity involving sums of squares of spherical Bessel functions; it is easy to verify this relation through terms of order Q^4, but we have not sought an independent derivation.

VII. DISCUSSION

This work has shown how the known hydrodynamic amplitudes [11] for a dilute condensed Bose gas in a spherical harmonic trap can provide the corresponding Bogoliubov spatial amplitudes for the quantum-mechanical field operators, including their absolute normalization. These normalized amplitudes in turn determine several important physical quantities, such as the excitation of each normal mode, both in the ground state and at low temperatures ($T \ll T_0$), and the dynamic structure factor that describes the inelastic scattering of a weakly interacting probe that couples to the density fluctuations of the Bose condensate. The hydrodynamic amplitudes are accurate only for low-lying modes, for their derivation neglects the quantum-mechanical kinetic energy that becomes increasingly important at short wavelengths. Thus our estimate of the total condensate depletion involves a cut-off that explicitly omits all the high-lying normal modes.

As noted by Singh and Rokhsar [29] and Stringari [11], the exact eigenfrequencies of the lowest dipole mode $l = 1$ for an anisotropic harmonic trap coincide with the bare oscillator frequencies; numerical work by several groups [29–33] has confirmed this conclusion for moderate values of N_0. The Appendix contains an analytical proof in the Bogoliubov approximation; it provides an explicit construction of the lowest dipole states for any solution of the GP equation, including those containing one or more vortices.

ACKNOWLEDGMENTS

We are grateful to S. Bahcall, M. Cole, A. Griffin, and S. Stringari for valuable comments and suggestions. This work was supported in part by the National Science Foundation, under Grants No. DMR 94-21888 and DMR 91-57414.

APPENDIX: DIPOLE MODE

Recently, the collective excitation spectrum of harmonically confined Bose gases has been calculated by several groups [11,29–33]. It has been noted [11,29] that these spectra contain a trio of exact collective modes that correspond to the simple-harmonic oscillation of the center of mass of the condensate. If the interacting condensate is displaced without deformation, the interparticle interactions are unchanged. Thus, the system experiences a restoring force that is simply linear in the displacement, with spring constant equal to that of the bare trap. There is one such mode for each of the three Cartesian directions.

In this Appendix, we construct the exact many-body raising operator that creates these "dipole" or "sloshing" modes and demonstrate the independence of their frequencies on the interparticle interactions. Since the collective modes of the dilute Bose gas are expected to be well-described by the Bogoliubov approximation, it is interesting to confirm that the dipole modes are in fact unrenormalized in this approximation. We therefore construct the exact solutions of the Bogoliubov equations that correspond to the dipole modes. These may be useful points of comparison with numerical calculations of the Bogoliubov spectrum. Finally, we examine the form of these modes in the Thomas-Fermi approximation [8], which is relevant for large condensates.

Definitions.

Consider bosons of mass m confined to a three-dimensional, harmonic potential with spring constants $m\omega_\alpha^2$, where $\alpha = x$, y, and z labels the three cartesian directions. The corresponding bare trap frequencies are ω_α. The (one-body) Hamiltonian of a single particle in the trap is then

$$\mathcal{H}_0 \equiv \sum_\alpha \left(\frac{p_\alpha^2}{2m} + \tfrac{1}{2} m \omega_\alpha^2 r_\alpha^2 \right), \tag{A1a}$$

or, equivalently,

$$\mathcal{H}_0 = \sum_\alpha \hbar\omega_\alpha (a_\alpha^\dagger a_\alpha + \tfrac{1}{2}), \tag{A1b}$$

where we introduce the usual raising and lowering operators

$$a_\alpha \equiv \frac{1}{\sqrt{2}} \left(\frac{x_\alpha}{d_\alpha} + d_\alpha \frac{\partial}{\partial x_\alpha} \right), \tag{A2a}$$

$$a_\alpha^\dagger \equiv \frac{1}{\sqrt{2}} \left(\frac{x_\alpha}{d_\alpha} - d_\alpha \frac{\partial}{\partial x_\alpha} \right), \tag{A2b}$$

and (as above) $d_\alpha \equiv \sqrt{\hbar/m\omega_\alpha}$. The operators a_α and $a_\alpha^\dagger$ obey Bose commutation relations, and they act on one-body states. They satisfy the familiar relation

$$[\mathcal{H}_0, a_\alpha^\dagger] = \hbar\omega_\alpha a_\alpha^\dagger \tag{A3}$$

which shows that $a_\alpha^\dagger$ is a raising operator of the noninteracting system.

Let $V(\mathbf{r} - \mathbf{r}')$ be the two-body interaction potential between the particles. The many-body Hamiltonian is then

$$\mathcal{H} = \sum_{i=1}^N \mathcal{H}_{0i} + \frac{1}{2} \sum_{i \neq j}^N V(\mathbf{r}_i - \mathbf{r}_j), \tag{A4}$$

where the index i and j labels individual particles, and N is the total particle number. For bosons, we consider only states that are symmetric under interchange of particle labels.

Dipole-mode creation operator

We claim that the (symmetric) operator

$$A_\alpha^\dagger \equiv \sum_{i=1}^N a_{\alpha i}^\dagger \tag{A5}$$

is a raising operator for the many-body Hamiltonian $\mathcal{H}$. That is,

$$[\mathcal{H}, A_\alpha^\dagger] = \hbar\omega_\alpha A_\alpha^\dagger. \tag{A6}$$

Thus if $|G\rangle$ is the exact many-body ground state of the interacting system, then $A_\alpha^\dagger |G\rangle$ is an *exact* excited state with excitation energy $\hbar\omega_\alpha$. Repeatedly applying $A_\alpha^\dagger$ to any exact eigenstate of $\mathcal{H}$ creates an equally spaced ladder of exact excited states. [Note that $(A_\alpha^\dagger)^2$ creates two quanta of the same elementary excitation and does not yield a distinct new elementary excitation itself.]

The proof is straightforward. The commutator Eq. (A6) is

$$[\mathcal{H}, A_\alpha^\dagger] = \sum_{ij} [\mathcal{H}_{0i}, a_{\alpha j}^\dagger] + \tfrac{1}{2} \sum_{ijk} [V_{ij}, a_{\alpha k}^\dagger]. \tag{A7}$$

The first set of commutators is easily evaluated using Eq. (A3) and gives $\hbar\omega_\alpha \sum_i a_{\alpha i}^\dagger = \hbar\omega_\alpha A_\alpha^\dagger$. The second set of commutators vanishes identically, since the terms cancel in pairs.

This operator $A_\alpha^\dagger$ makes good physical sense. Beginning from any exact many-body eigenstate, we raise each particle in turn by a single quantum, and then superimpose the resulting states to produce a symmetric wave function. The proof is similar to the demonstration that the cyclotron frequency of an interacting, translationally invariant system is unrenormalized, *i.e.,* Kohn's theorem [34].

Dipole mode in the Bogoliubov approximation.

Is the same dipole mode also present as an exact solution of the Bogoliubov equations for harmonically trapped bosons? The answer to this question is not completely obvious, since the Bogoliubov approximation assumes the existence of a condensate, which provides a provides a preferred reference frame (usually, but not necessarily, at rest). We will show that the spectrum of the dilute Bose gas in the Bogoliubov approximation possesses *exact* excited states that are simply related to the dipole modes discussed above.

Let $\Psi(\mathbf{r})$ be the condensate wave function of the interacting system, which is an exact solution of the Gross-Pitaevskii equation [Eq. (5)]:

$$(\mathcal{H}_0 + g|\Psi|^2)\Psi = \mu\Psi, \tag{A8}$$

where $g = 4\pi a\hbar^2/m$ characterizes the strength of the interparticle potential and μ is the chemical potential. We claim that the excited state

$$\begin{pmatrix} u_\alpha(\mathbf{r}) \\ v_\alpha(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} a_\alpha^\dagger \Psi(\mathbf{r}) \\ a_\alpha \Psi^*(\mathbf{r}) \end{pmatrix} \tag{A9}$$

is then an exact solution of the Bogoliubov equations with excitation frequency equal to the bare trap frequency ω_α. There is one such mode for each coordinate direction.

Note that for the noninteracting case ($g = 0$), a_α annihilates the condensate wave function Ψ, which is then simply the ground state Ψ_0 of the harmonic potential. Equation (A9) then reduces to

$$\begin{pmatrix} u_\alpha(\mathbf{r}) \\ v_\alpha(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} a_\alpha^\dagger \Psi_0(\mathbf{r}) \\ 0 \end{pmatrix} \qquad \text{(noninteracting)}. \tag{A10}$$

As expected, exact quasiparticle states are created by adding a particle to the first excited state of the trap.

It is straightforward to prove that Eq. (A9) is an exact solution of the Bogoliubov equations for *any* coupling strength g. The proof proceeds by the explicit demonstration that the u_α, v_α of Eq. (A9) satisfy the coupled Bogoliubov equations (7). We use the elementary properties of a_α and $a_\alpha^\dagger$, and the fact that Ψ satisfies the Gross-Pitaevskii equation [Eq. (A8)]. The argument explicitly relies on the harmonic character of the trap $V(\mathbf{r})$, with $a_\alpha^\dagger$ and a_α as raising and lowering operators for the single-particle problem; it cannot be extended to problems without a simple ladder of noninteracting levels.

We now confirm that the first of the two coupled Bogoliubov equations Eq. (7a) is satisfied by our proposed solution Eq. (A9); the second equation Eq. (7b) is simply the complex conjugate of the first. Substituting Eq. (A9) into Eq. (7a), we need to show that

$$(\mathcal{H}_0 + g|\Psi|^2 - \mu)\, a_\alpha^\dagger\Psi + g|\Psi|^2 a_\alpha^\dagger\Psi - g\Psi^2 a_\alpha\Psi^* \stackrel{?}{=} \hbar\omega_\alpha a_\alpha^\dagger\Psi. \tag{A11}$$

Multiplying the Gross-Pitaevskii equation (5) by $a_\alpha^\dagger$ yields

$$a_\alpha^\dagger(\mathcal{H}_0 + g|\Psi|^2 - \mu)\Psi = 0. \tag{A12}$$

Subtracting Eq. (A12) from Eq. (A11) then reduces our problem to showing that

$$[\mathcal{H}_0, a_\alpha^\dagger]\Psi + g[\,|\Psi|^2, a_\alpha^\dagger]\Psi + g|\Psi|^2 a_\alpha^\dagger\Psi - g\Psi^2 a_\alpha\Psi^* \stackrel{?}{=} \hbar\omega_\alpha a_\alpha^\dagger\Psi. \tag{A13}$$

From Eq. (A3), the first commutator is simply $[\mathcal{H}_0, a_\alpha^\dagger] = \hbar\omega_\alpha a_\alpha^\dagger$, which cancels the right hand side of Eq. (A13).

Finally, our task is reduced to showing that

$$[\,|\Psi|^2, a_\alpha^\dagger]\,\Psi + |\Psi|^2 a_\alpha^\dagger\Psi - \Psi^2 a_\alpha\Psi^* \stackrel{?}{=} 0; \tag{A14}$$

this result is easy to confirm with the explicit form of $a_\alpha^\dagger$ and a_α in Eqs. (A2a) and (A2b).

Note that this construction is entirely general. It makes no assumption that Ψ is real, and thus holds for *any* solution of the Gross-Pitaevskii equation (5), including those describing vortices [35]. For any self-consistent condensate, the lowest dipole modes will have the bare oscillation frequencies.

Nature of the dipole mode.

Excitation of the dipole mode leads to an oscillatory density-fluctuation amplitude that is one of the normal modes described in Eq. (23). For simplicity, we consider explicitly only the case of a condensate with real Ψ, *i.e.,* a stationary condensate.

Equations (23) then become

$$\begin{aligned}\delta\rho_\alpha &= \Psi\left(u_\alpha - v_\alpha\right) = \Psi\big(a_\alpha^\dagger\Psi - a_\alpha\Psi\big)\\ &= \sqrt{2}\Psi d_\alpha \frac{\partial\Psi}{\partial r_\alpha} \propto \frac{\partial n_0}{\partial r_\alpha}.\end{aligned} \tag{A15}$$

This expression confirms that the quasiparticle mode created by the linear combination of $a_\alpha^\dagger$ and a_α corresponds to a uniform displacement of the condensate in the αth direction. Similarly, the velocity potential associated with this condensate motion is [see Eq. (23)]

$$\begin{aligned}\delta\Phi_\alpha &= \frac{\hbar}{2mi\Psi}\left(u_\alpha + v_\alpha\right) = \frac{\hbar}{2mi\Psi}\left(a_\alpha^\dagger\Psi + a_\alpha\Psi\right)\\ &= \frac{-i\hbar}{\sqrt{2}m}\,\frac{r_\alpha}{d_\alpha};\end{aligned} \tag{A16}$$

the corresponding velocity $\mathbf{v} = \nabla\delta\Phi_\alpha$ lies along the displacement with constant amplitude and is $\frac{1}{2}\pi$ out of phase relative to the density fluctuation Eq. (A15) due to the factor of i.

Thomas-Fermi approximation

Finally, we examine the dipole mode in the Thomas-Fermi limit, where the Gross-Pitaevskii equation can be solved exactly. For simplicity we consider an isotropic trap, although the same results hold for anisotropic traps of the sort used in Refs. [29,30]. The condensate wave function is then given by

$$\Psi_{TF}(\mathbf{r}) \propto \sqrt{R_0^2 - r^2}, \tag{A17}$$

where $R_0 \propto N_0^{1/5}$ is the size of the condensate. Using Eq. (24) and the operators from Eqs. (A2), we find

$$u_\alpha(\mathbf{r}) = a_\alpha^\dagger\Psi(\mathbf{r}) \propto r_\alpha\left[\sqrt{R_0^2 - r^2} + \frac{1}{\sqrt{R_0^2 - r^2}}\right] \tag{A18a}$$

$$v_\alpha(\mathbf{r}) = a_\alpha\Psi(\mathbf{r}) \propto r_\alpha\left[\sqrt{R_0^2 - r^2} - \frac{1}{\sqrt{R_0^2 - r^2}}\right] \tag{A18b}$$

Although $\delta\rho$ and $\delta\Phi$ remain finite everywhere, both both u_α and v_α diverge at the perimeter of the condensate. This pathology evidently arises from the extreme Thomas-Fermi limit, for it reflects the singular behavior of Ψ_{TF} at the condensate boundary. Any finite interparticle interaction strength g renders the condensate wave function Ψ differentiable everywhere, and the exact Ψ vanishes smoothly for $r \to \infty$ [21]; then u_α and v_α also vanish smoothly. Despite the separate divergences, the approximate two-component Bogoliubov state in the TF limit in Eq. (A18) remains normalizable, since we require only that $\int_0^\infty r^2\,dr\,\left(|u_\alpha|^2 - |v_\alpha|^2\right) = 1$.

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[1] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, Science **269**, 198 (1995).

[2] K. B. Davis, M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, Phys. Rev. Lett. **75**, 3969 (1995).

[3] C. C. Bradley, C. A. Sackett, and R. G. Hulet, Phys. Rev. Lett. **78**, 985 (1997).

[4] D. S. Jin, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, Phys. Rev. Lett. **77**, 420 (1996).
[5] M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. M. Kurn, D. S. Durfee, C. G. Townsend, and W. Ketterle, Phys. Rev. Lett. **77**, 988 (1996).
[6] N. N. Bogoliubov, J. Phys. (USSR) **11**, 23 (1947).
[7] For additional early treatments that clarified the role of the pseudopotential, see T. D. Lee and C. N. Yang, Phys. Rev. **105**, 1119 (1957) and T. D. Lee, K. Huang, and C. N. Yang, Phys. Rev. **106**, 1135 (1957).
[8] G. Baym and C. J. Pethick, Phys. Rev. Lett. **76**, 6 (1996).
[9] A. L. Fetter, Ann. Phys. (N. Y.) **70**, 67 (1972).
[10] The analogous self-consistent equations for a superconductor are now generally known as the Bogoliubov-de Gennes equations [see, for example, P. G. de Gennes, *Superconductivity of Metals and Alloys* (Benjamin, NY, 1966), Chap. 5].
[11] S. Stringari, Phys. Rev. Lett. **77**, 2360 (1996).
[12] A. L. Fetter, Phys. Rev. A **53**, 4245 (1996).
[13] W.-C. Wu and A. Griffin, Phys. Rev. A **54**, 4204 (1996).
[14] E. P. Gross, Nuovo Cimento **20**, 454 (1961); J. Math. Phys. **46**, 137 (1963).
[15] L. P. Pitaevskii, Zh. Eksp. Teor. Fiz. **40**, 646 (1961); Sov. Phys.–JETP **13**, 451 (1961).
[16] The relevant scattering theory (in the context of many-body physics) is reviewed in A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, NY, 1971), Secs. 11, 22, and 35.
[17] For example, the addition of repulsive interactions completely alters the density profile from that associated with the ideal single-particle ground state. See, *e.g.*, T. T. Wu, J. Math. Phys. **2**, 105 (1961), which shows that a Bose condensate in a one-dimensional box of length L with rigid walls is exactly soluble for $0 < a \ll \min(\xi, L)$, independent of the ratio ξ/L, explicitly illustrating the alteration in the condensate density from "ideal" to "dilute" as ξ/L changes from large to small.
[18] M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. M. Kurn, D. S. Durfee, and W. Ketterle, Phys. Rev. Lett. **77**, 416 (1996).
[19] M. Edwards and K. Burnett, Phys. Rev. A **51**, 1382 (1995).
[20] P. A. Ruprecht, M. J. Holland, K. Burnett, and M. Edwards, Phys. Rev. A **51**, 4704 (1995).
[21] F. Dalfovo, L. P. Pitaevskii, and S. Stringari, Phys. Rev. A **54**, 4213 (1996).
[22] See, for example, Ref. [16], Secs. 35 and 55.
[23] *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, edited by M. Abramowitz and I. A. Stegun (Nat. Bur. Stds., Washington, DC, 1968), Chaps. 15 and 22.
[24] See, for example, Ref. [16], Sec. 18.
[25] A. L. Fetter and D. L. Feder, unpublished.
[26] D. Pines and P. Nozières, *The Theory of Quantum Liquids*, Vol. I (Benjamin, NY, 1966), Chap. 2.
[27] N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Holt, Rinehart and Winston, NY, 1976), App. N.
[28] See, for example, Ref. [23], Sec. 10.1.
[29] K. G. Singh and D. Rokhsar, Phys. Rev. Lett. **77**, 1667 (1996).
[30] M. Edwards, P. A. Ruprecht, K. Burnett, R. J. Dodd, and C. W. Clark, Phys. Rev. Lett. **77**, 1671 (1996).
[31] M. Edwards, R. J. Dodd, C. W. Clark, and K. Burnett, J. Res. NIST **101**, 553 (1996).
[32] P. A. Ruprecht, M. Edwards, K. Burnett, and C. W. Clark, Phys. Rev. A **54**, 4178 (1996).
[33] L. You, W. Hoston, M. Lewenstein, and K. Huang, unpublished.
[34] W. Kohn, Phys. Rev. **123**, 1242 (1961).
[35] R. J. Dodd, K. Burnett, M. Edwards, and C. W. Clark, cond-mat/9610093, unpublished.